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Thermally Fluctuating Inhomogeneous Superfluid State of Strongly Interacting Fermions in an Optical Lattice

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The presence of attractive interaction between fermions can lead to pairing and superfluidity in an optical lattice. The temperature needed to observe superfluidity is about a tenth of the tunneling energy in the optical lattice, and currently beyond experimental reach. However, at strong coupling the precursors to global superfluidity should be visible at achievable temperatures, in terms of fluctuating domains with strong pairing correlations. We explore this regime of the attractive two dimensional fermion Hubbard model, in the presence of a confining potential, using a new Monte Carlo technique. We capture the low temperature inhomogeneous superfluid state with its unusual spectral signatures but mainly focus on the experimentally accessible intermediate temperature state. In this regime, and for the trap center density we consider, there is a large pairing amplitude at the center, spatially correlated into domains extending over several lattice spacings. We map out the thermal evolution of the local density, the double occupancy, the pairing correlations, and the momentum distribution function across this phase fluctuation window.

The development of optical lattice methods for ultracold atoms has opened a new vista in the study of correlated systems [1–4], allowing clean controllable realisations of strongly interacting quantum lattice models. Experimental achievements include the realisation of the superfluid (SF) to Mott insulator transition [5] in the Bose Hubbard model, and, for repulsive fermions, the observation of Fermi surface [6], and the Mott insulating phase [7, 8]. For attractive interactions, there has been the evidence of superfluidity [9], a possible FFLO state [10], and anomalous expansion of the Fermi gas [11]. The realisation of an antiferromagnetic state [12, 13] in the repulsive Hubbard model and of superfluidity in the attractive model [14] is still awaited. The problem is with the achievable temperature [15].

Techniques available to date can reduce the entropy, S, per particle of a Fermi gas to $\sim \log_e 2 \approx 0.7$. The associated temperature is $\mathcal{O}(t)$, where t is the tunneling energy between neighbouring wells in the periodic potential. The observation of superfluidity in the attractive Hubbard model will require cooling to $k_BT/t \sim 0.1$. The corresponding entropy is $S \sim 0.1$ [15], almost an order of magnitude below what is currently achievable. What signatures would one expect of attractive interactions at accessible temperatures? At weak coupling the state above T_c is a normal Fermi liquid but at strong coupling a large pairing amplitude survives to $T \gg T_c$ and entropy levels $S \sim \log_e 2$. This is an *inhomogeneous, thermally fluctuating, short range correlated state*, with striking measurable properties.

In this paper we solve the attractive ('negative U') Hubbard model on large two dimensional lattices in the presence of a confining potential. Our main results are the following: (i) We access the superfluid ground state, the thermal transition, and a wide temperature window over which the Fermi system has large pairing amplitude but no global phase coherence. (ii) We illustrate how fluctuating filamentary 'superfluid' regions survive far above T_c, to temperatures $k_BT/t \sim \mathcal{O}(1)$, and leave signatures on the spatial patterns and spectral features. We demonstrate these using a new method that handles the strong coupling non-perturbatively and treats the spatial inhomogeneity and strong thermal fluctuations exactly.

We study the attractive Hubbard model in the presence of a harmonic potential V_i in two dimensions:

$$H = -t \sum_{\langle ij \rangle \sigma} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i\sigma} (V_i - \mu) n_{i\sigma} - U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (1)$$

The first term denotes the nearest neighbour tunneling amplitude of fermionic atoms on the optical lattice, the confining potential has form $V_i = V_0(x_i^2 + y_i^2)$, μ is the chemical potential, and $U > 0$ is the strength of attractive on-site interaction. x_i and y_i are measured in units of lattice spacing a_0.

The spatial variation in mean value, and the thermal fluctuation about the mean, of the amplitude and phase of the order parameter are crucial in describing the physics of this system. Unbiased calculations in the homogeneous limit employ determinantal quantum Monte Carlo [15–17] (DQMC) to access finite temperature properties, but are typically limited to 10×10 lattices. That is inadequate to clarify the interplay of correlation effects and inhomogeneity.

We use a strategy used earlier on moderately sized systems [18, 19], augmented now by a 'traveling cluster' (TCA) [20] Monte Carlo technique that readily allows access to system size $\sim 32 \times 32$. We first decouple the Hubbard term in the pairing channel by using the Hubbard-Stratonovich (HS) transformation. We use the static HS (sHS) approximation [18], *i.e*, retain spatial fluctuations of HS fields but ignore the time dependence. This leads to the following effective Hamiltonian:

$$H_{eff} = H_0 + \sum_i (\Delta_i c^{\dagger}_{i\uparrow} c^{\dagger}_{i\downarrow} + \Delta^{\star}_i c_{i\downarrow} c_{i\uparrow}) + \sum_i \frac{|\Delta_i|^2}{U} \quad (2)$$

where $H_0 = -t\sum_{\langle ij\rangle\sigma} c^\dagger_{i\sigma}c_{j\sigma} + \sum_{i\sigma}(V_i-\mu)n_{i\sigma}$ and $\Delta_i = |\Delta_i|e^{i\theta_i}$ is a complex scalar *classical* field. This model allows fluctuations in both the amplitude and phase of the pairing field Δ_i, and the fermions propagate typically in an inhomogeneous background defined by Δ_i.

To obtain the ground state, and in general configurations $\{|\Delta_i|, \theta_i\}$ that follow the distribution $P\{|\Delta_i|, \theta_i\} \propto Tr_{c,c^\dagger} e^{-\beta H_{eff}}$, we use the Metropolis algorithm to update the $|\Delta|$ and θ variables. This involves solution of the Bogoliubov-de Gennes (BdG) equation [21] for each attempted update. For equilibriation we use the traveling cluster algorithm [20], diagonalising the BdG equation on a 8×8 cluster around the update site. Global properties like pairing field correlation, quasiparticle density of states, *etc*, are computed via solution of the BdG equation on the *full system* for equilibrium configurations.

We explored the system at $U/t = 2,\ 6,\ 12$ and the maximum (system corner) potential $V_c \sim V_0{*}2{*}(L/2)^2 = U/2,\ U,\ 2U$, where the system size is $L \times L$. This enables us to systematically study the evolution from weak to strong coupling, as well as weak to strong confinement. We focus on the strong coupling, strong inhomogeneity case, $U = 12,\ V_c = 24$ in this paper and will discuss the larger parameter set separately [22].

In the absence of the confining potential the model is known [16, 17] to have a superfluid ground state for all densities $n \neq 1$, while at $n = 1$ there is the coexistence of superfluid and density wave (DW) correlations. The SF ground state away from $n = 1$ evolves [23] from a Bardeen-Cooper-Schrieffer (BCS) state at $U/t \ll 1$ to a Bose-Einstein condensed (BEC) state of 'molecular pairs' at $U/t \gg 1$. The ground state can be reasonably accessed within mean field theory (MFT) but the finite temperature predictions of MFT becomes increasingly inaccurate with increase in U [24]. This is due to the separation of scales between 'pair formation' temperature, $T_f \sim \mathcal{O}(U)$, and pair condensation, *i.e*, superfluidity, which is $T_c \sim t^2/U$. MFT captures T_f but wrongly identifies it with the superfluid transition.

For $U/t \lesssim 1$, the state at $T > T_c$ is an uninteresting weakly correlated Fermi liquid. As U/t increases, T_c (in two dimensions) peaks at $U/t \approx 5$, while T_f continues to grow. A wide 'non-Fermi liquid' window opens up between T_c and T_f, and the system behaves like a (hard-core) Bose liquid [24] for low temperature and $U/t \gg 1$. In this $U \gg t$ regime, increasing T leads to gradual dissociation of the 'bosons', and paired and unpaired fermions exist in equilibrium.

The confining potential promotes an inhomogeneous density profile [25], with a peak at the trap center. If the average density near trap center is $n = 1$, it can lead to a local DW pattern [26, 27] while the SF would show up away from the center where $n < 1$. If the total particle number is sufficiently small so that even the central density is < 1, the entire system is an inhomogeneous SF

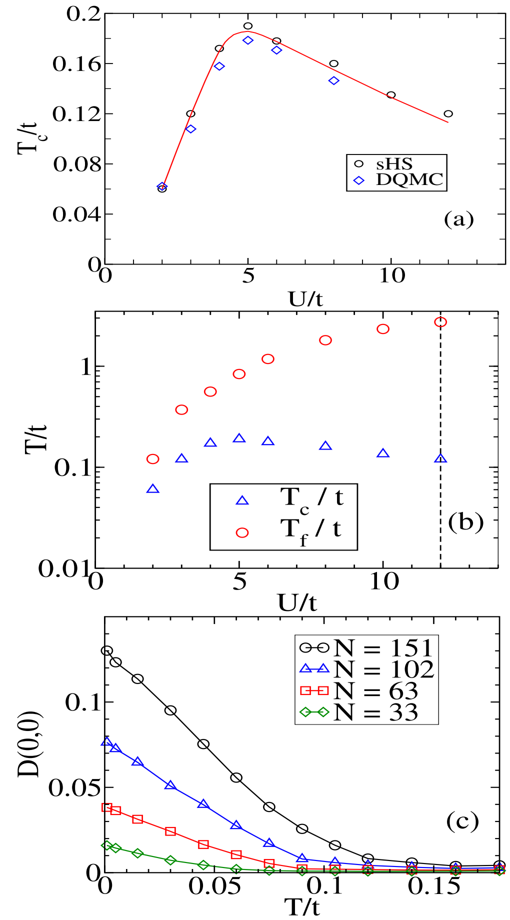

FIG. 1: Colour online: (a). Comparison of the $T_c(U)$ at $n = 0.7$ on 'flat' 10×10 lattices, obtained by two different techniques, the DQMC and our static HS approximation. (b). Schematic phase diagram in the flat case, indicating the window between the SF transition (T_c) and 'pair formation' scale (T_f) that grows with increasing U. The y scale is logarithmic to include the widely different scales of T_c and T_f. The vertical dotted line indicates the T dependence that we explore. (c). The growth of superfluid correlations at $U/t = 12$, $V_c/t = 24$, as indicated by the zero momentum component of the pairing field correlation. Both the onset temperature and $T = 0$ value are suppressed at lower N. System size 32×32.

at low temperature. In our strong confinement problem we will focus on the case where the total particle number $N \approx 150$. This leads to a trap center density $n = 0.9$, optimising the T_c for our choice of U and V_c. For weaker confinement a larger N can be used.

Fig.1.(a) compares the result of full DQMC calculation [15] with that of the sHS scheme implemented via TCA. The comparison on 10×10 lattices, with $V_0 = 0$ and $n \sim 0.7$, shows that our method captures the overall trend in $T_c(U)$ and is even quantitatively accurate. In our understanding the agreement is due to the inclusion of the key thermal phase fluctuations within the static HS theory. This gives us confidence in the method when applied to large lattices and the presence of a potential.

Fig.1.(b) highlights the two key scales from the $V_0 = 0$ problem, at $n = 0.7$, that are relevant for us: (i) the non-monotonic T_c scale whose maximum is roughly $0.18t$ and, (ii) the pair formation temperature T_f as defined below. We know that the pair binding energy is $\mathcal{O}(U)$ when U/t is large. To fix the prefactor, we *define* $T_f = 2\Delta_g(0)/3.5$, where $2\Delta_g(0)$ is the $T = 0$ gap in the quasiparticle spectrum. For $U/t \ll 1$, both superfluidity and the pairing amplitude vanish when $T = 2\Delta_g(0)/3.5$ and $T_c = T_f$ by definition. At strong coupling $2\Delta_g \sim U$, so $T_f \propto U$.

Fig.1.(c) shows the growth in the $\mathbf{Q} = \{0, 0\}$ component of the pairing field correlations, $D(\mathbf{Q}) = \sum_{ij} |\Delta_i||\Delta_j| cos(\theta_i - \theta_j) e^{i\mathbf{Q}.(\mathbf{r}_i - \mathbf{r}_j)}$. This is non zero when the amplitude $|\Delta_i|$ is finite over some region and the phases θ_i are correlated. This in turn promotes a non zero value of $\langle\langle c^\dagger_{i\uparrow} c^\dagger_{i\downarrow}\rangle\rangle$ and a finite value for $\chi(ij, T) = \langle\langle c^\dagger_{i\uparrow} c^\dagger_{i\downarrow} c_{j\downarrow} c_{j\uparrow}\rangle\rangle$. We therefore use $D(\{0, 0\}, T)$ as indicator of the SF transition. This is shown for choices of particle number N that lead to trap center density $n_i \leq 1$. The T_c scale, at $N \sim 150$ is roughly $0.12t$. At lower N the onset temperatures are lower and the strength of pairing field correlation at $T = 0$ is also smaller.

Accessible temperatures are still $\gg T_c^{\max} \sim 0.18t$ so one would have to look for non trivial interaction effects at $T > T_c$. At weak coupling the $T > T_c$ state is uninteresting. However, for $U/t \gtrsim 5$, the window between T_c and T_f is wide and well accessible with present cooling techniques. We highlight the particularly wide window at $U = 12$ that reaches from $T/t \sim 0.1 - 3$.

We chose μ such that the maximum density, which occurs at the trap center, was always less than 1, and the ground state of the system does not involve any DW order. Our ground state is always an inhomogeneous SF. Fig.2, left column, shows the spatial patterns in the 'ground state' ($T = 0.001t$). For our choice of μ, the density at the center is ~ 0.9. The double occupancy $d_i = \langle\langle n_{i\uparrow} n_{i\downarrow}\rangle\rangle$ follows a similar profile and is almost *double* the noninteracting value $(n_i/2)^2$ due to the strong interaction. The pairing field amplitude is also largest at the center (in the uniform case the pairing amplitude increases with n from $n = 0$ to $n \lesssim 1$). The phase correlations are near perfect in the ground state, as the bottom row, left column indicates.

The central and right column in Fig.2 highlights the thermal evolution, with the results averaged over 40 configurations. The middle column is for $T/t = 0.09$, and the right for $T/t = 0.50$. The global order parameter for superfluidity vanishes at $T/t \sim 0.12$ but, as expected at large U/t, the pairing amplitude still survives. From $T = 0.001t$ (left column) to $T \sim T_c$ (middle column) there is no significant change in the density pattern, the double occupancy, or the pairing amplitude. The pairing correlation (bottom row) is still dominantly positive at $T/t = 0.09$ but with hints of small (minority) domains.

At the highest temperature, $T = 0.50t$, right column,

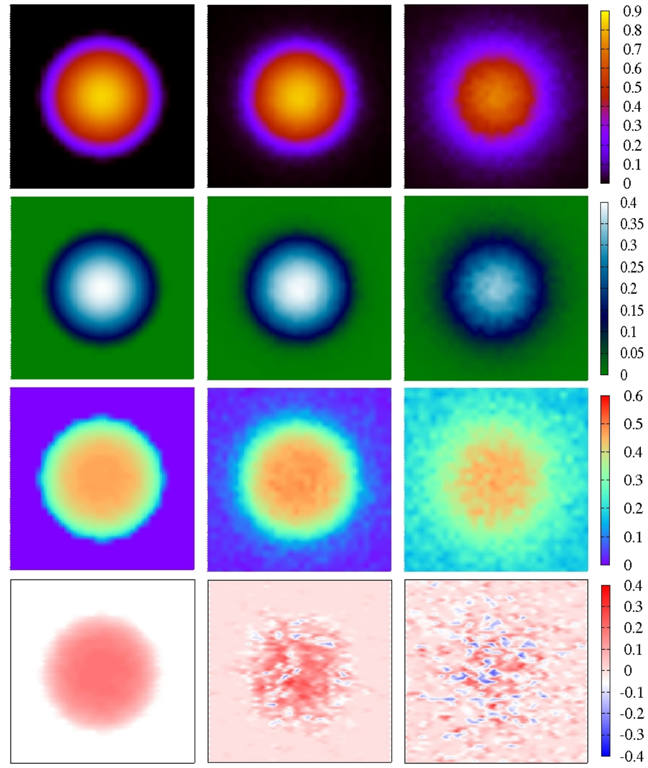

FIG. 2: Colour online: Temperature dependence of spatial patterns. The results are all for $N \approx 150$. The first column is for $T/t = 0.001$ (the ground state), the second column for $T/t = 0.090$ (roughly below T_c) and the third column at $T/t = 0.50$, deep in the fluctuating regime. The first row shows n_i, the second shows the double occupancy d_i, the third shows the pairing field magnitude $|\Delta_i|$, the fourth shows the nearest neighbour pairing field correlation. System size 32×32.

where we expect the average entropy to be ~ 0.5 per particle, the n_i pattern is significantly broader and the associated d_i is more diffuse (with a slightly lower trap center value). The pairing amplitude is still significant, although the averaging has not completely restored the circular symmetry. The pairing correlation reveals a strong short range feature, and a filamentary pattern with lengthscale $\sim 5a_0$. The correlations are stronger, overall, near the central part, but now have some strength towards the periphery also due to the density broadening.

A direct measure of the correlated phase is the quasiparticle density of states (DOS), $N(\omega) = \langle\langle \sum_n \delta(\omega - E_n)\rangle\rangle$, shown in Fig.3 for $T/t = 0.001,\ 0.25,\ 0.50$. E_n are the BdG eigenvalues in the equilibrium Δ_i background. At $T = 0.001$ there are three noteworthy features: (i) the pairing gap $\approx U$, (ii) the coherence peaks at the gap edge, reminiscent of 'flat' systems, and (iii) the 'spiky' features that arise from the quantisation of energy levels in this 'stiff' trap. We have checked that the sharp levels survive, but become more regularly spaced, even in the non-interacting case. It is now possible to measure the spectral function via photoemission [28] in cold atom

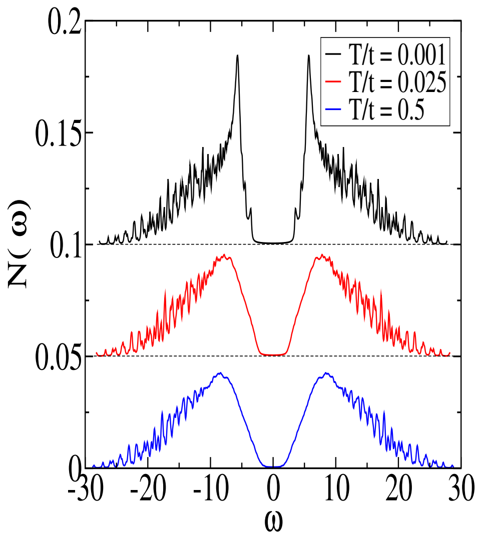

FIG. 3: Colour online: Quasiparticle density of states for $T/t = 0.001,\ 0.25,\ 0.50$. $T_c \approx 0.12$, so the results are approximately for $T = 0,\ 2.5T_c$ and $5T_c$. The gap and the spiky features survive over this temperature window and are related, respectively, to 'preformed pairs' and the level quantisation due to the confining potential. System size 32×32.

experiments.

We observed that with increasing T the coherence features get wiped out and vanish by the time $T \sim T_c/2$. The pairing gap, however, survives but with two modifications. The region over which $N(\omega) = 0$ now shrinks (the gap lessens) but with the loss of the coherence peaks there is a loss in band edge spectral weight. The quantised features still survive but are more diffuse. This gapped spectrum is visible even at $T/t = 0.50$, like the Mott gap in the positive U Hubbard model.

Let us discuss the momentum distribution function $n(k_x, k_y)$, Fig.4, as the final signature of correlation physics. This can be measured from the velocity distribution of the gas by switching off the trap. The left panel in Fig.4 shows $n(k_x, k_y)$ for the ground state of the

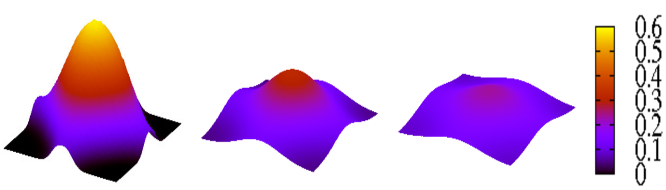

FIG. 4: Colour online: Momentum distribution function, $n(k_x, k_y)$. The left panel shows the $n(k_x, k_y)$ for a *non-interacting* fermion gas in the trap, with $N = 150$ and $T = 0$. Although there is expectedly no sharp 'Fermi surface', due to the background potential, $n(k_x, k_y)$ has strong momentum dependence. Middle panel is for trapped interacting fermions at $T/t = 0.001$. Right panel is the trapped interacting system at $T/t = 0.50$

non-interacting trapped gas (at same N). While there is no Fermi surface (FS) there is a strong momentum dependence. $n(k_x, k_y)$ is very distinct in the interacting case: flat and broad with only a weak central peak in the ground state, and essentially flat at $T/t = 0.50$. Tuning the Feshbach resonance across the BCS-BEC crossover should observe this broadening.

Conclusions: We have studied the attractive Hubbard model at strong coupling in the presence of a harmonic confining potential. Our non perturbative results highlight the destruction of global superfluid order at fairly low temperature but the survival of nanoscale fluctuating 'paired' regions to high temperature. They leave an imprint on the spectral density and momentum distribution which serve as precursors to global coherence.

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[1] D. Jaksch, *et al.*, Phys. Rev. Lett. **81**, 3108 (1998).
[2] T. Esslinger, Annual Review of Condensed Matter Physics, **1**, 129 (2010), arXiv:1007.0012.
[3] I. Bloch, Nature Physics **1** (2005) 23.
[4] D. Jaksch and P. Zoller, Ann. Phys. (NY) **315**, 52 (2005).
[5] M. Greiner, *et al.*, Nature **415**, 39 (2002).
[6] M. Kohl, *et al.*, Phys. Rev. Lett. **94**, 080403 (2005).
[7] U. Schneider, *et al.*, Science, **322**, 1520 (2008).
[8] R. Jordens, *et al.*, Nature, **455**, 204 (2008).
[9] J. K. Chin, *et al.*, Nature **443**, 961 (2006).
[10] Yean-an Liao, *et al.*, Nature, **467**, 567 (2010).
[11] L. Hackermuller, *et al.*, Science, **327**, 1621 (2010).
[12] E. V. Gorelik, *et al.*, Phys. Rev. Lett. **105**, 065301 (2010).
[13] S. Chiesa, *et al.*, Phys. Rev. Lett. **106**, 035301 (2011).
[14] W. Hofstetter, *et al.*, Phys. Fev. Lett. **89**, 220407 (2002).
[15] T. Paiva, *et al.*, Phys. Rev. Lett. **104**, 066406 (2010).
[16] R. T. Scalettar, *et al.*, Phys. Rev. Lett. **62**, 1407 (1989).
[17] A. Moreo and D. J. Scalapino, Phys. Rev. Lett. **66**, 946 (1991).
[18] Y. Dubi, *et al.*, Nature, **449**, 876 (2007).
[19] M. Mayr, G. Alvarez and E. Dagotto, Phys. Rev. Lett. **94**, 217001 (2005).
[20] S. Kumar and P. Majumdar, Eur. Phys. J. B, **50**, 571 (2006).
[21] P. G. de Gennes, *Superconductivity of metals and alloys*, Addison Wesley (1989).
[22] S. Datta, V. Singh and P. Majumdar, unpublished.
[23] P. Nozieres and S. Schmitt-Rink, J. Low. Temp. Phys. **59**, 195 (1985).
[24] For an early review, see R. Micnas, *et al.*, Rev. Mod. Phys. **62**, 113 (1990).
[25] T.-L. Dao, A. Georges, and M. Capone, Phys. Rev. B**76**, 104517 (2007).
[26] A. Koga, *et al.*, Phys. Rev. A**79**, 013607 (2009).
[27] M. Machida, *et al.*, Phys. Rev. A **74**, 053621 (2006).
[28] J. T. Stewart, J. P. Gaebler and D. S. Jin, Nature, **454**, 744 (2008).